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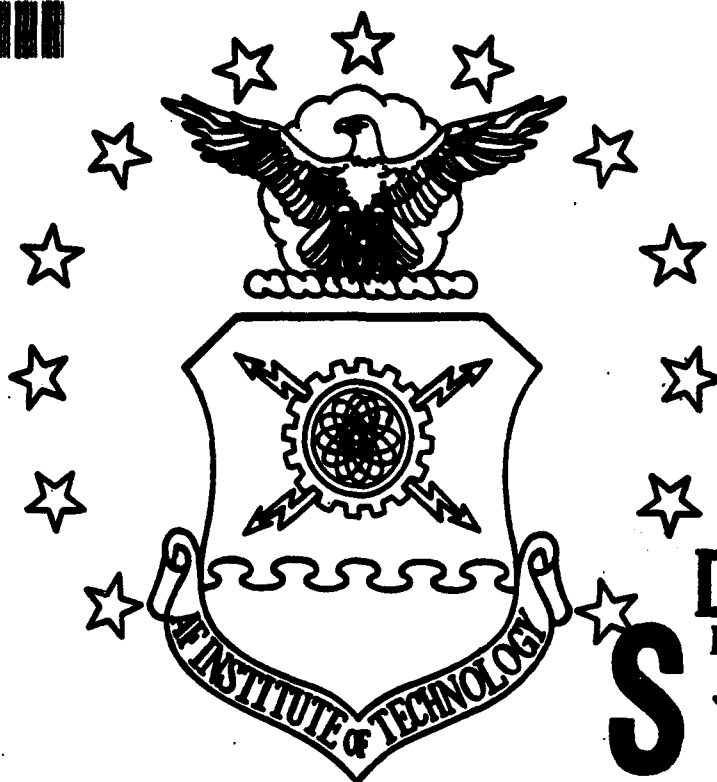
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ESTIMATING GROUNDWATER FLOW PARAMETERS
USING RESPONSE SURFACE METHODOLOGY

THESIS

Leo C. Adams, Captain, USAF

AFIT/GSO/ENS/94A-01

DEPARTMENT OF THE AIR FORCE
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THESIS

Presented to the Faculty of the Graduate School of Engineering

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In Partial Fulfillment of the

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Master of Science in Space Operations

Leo C. Adams, B.S.

Captain, USAF

April, 1994

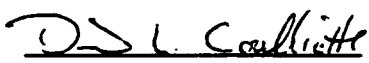| Accesion For		
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THESIS APPROVAL

Student: Captain Leo C. Adams   Class: GSO-93D

Thesis Title: Estimating Groundwater Flow Parameters Using
                 Response Surface Methodology

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Craig Adams

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ABSTRACT

This thesis examined the use of response surface methodology (RSM) as a parameter estimation technique in the field of groundwater flow modeling. Using RSM, an attempt was made to calibrate three hydraulic parameters (porosity, transverse permeability, and rate of recharge) of an existing two-dimensional, steady-state flow model. The model simulated groundwater flow for a portion of landfill 10 located on Wright-Patterson Air Force Base, Ohio. The model had previously been calibrated by graphical matching observed water-levels to predicted water-levels. Using the parameter values from the earlier calibration effort as a starting point, a central composite design was developed and the simulation executed at each design point. A residual sum of squares function was used as the calibration criteria and an empirical model of the error surface was developed. Of the three hydraulic parameters, only transverse permeability had a significant effect on the response. The regression model also indicated the response had a high degree of variability. A graph of the regression equation revealed no local optima within the design region indicating the initial parameter estimates may not have been warranted.

ESTIMATING GROUNDWATER FLOW PARAMETERS USING RESPONSE SURFACE METHODOLOGY

I. Introduction

Background

The demand for municipal, agricultural, and industrial use of groundwater, and concerns about groundwater contamination, have steadily grown over the years. In response, hydrologists and water resources personnel have searched for better ways to understand and manage groundwater systems. This search has led to the development of numerous groundwater flow and solute transport models. The majority of these models are simulation models implemented on computers. Generally, these simulation models include four categories of mathematical descriptions:

1. the relevant laws which govern the various processes inherent in the system;

2. the hydrogeology (aquifer configuration and parameters);

3. the external forces exerting on the system; and

4. the initial and boundary conditions of the system.

While the relevant laws are general principles that apply to every groundwater flow system, the parameters of the second, third, and fourth categories must be specified for the model to adequately characterize a particular system (Xiang and others, 1993:1661). Adequately determining these parameters is one of the most difficult aspects of groundwater flow modeling (Neuman, 1973:1006).

The process of estimating the model parameters to obtain a reasonable match between observed, site-specific data and model calculations is known as model calibration (Walton, 1992:35). Traditionally, model calibration has been done by manual trial-and-error and graphical matching techniques. In addition to being time consuming, these

methods are often very qualitative and leave the reliability of the model in question (Faust and Mercer, 1980:572). While several automated techniques have been developed to estimate parameters by optimizing an objective function, most practitioners still prefer the manual trial-and-error method (Anderson and Woessner, 1992:266).

One approach that may be useful in performing model calibration is response surface methodology (RSM). RSM consists of a set of techniques used in the empirical study of relationships between one or more responses and a group of input variables. These techniques include:

1. Designing a set of experiments that will yield adequate measurements of the response(s) of interest.

2. Determining a mathematical model that best fits the data collected from the experimental runs.

3. Determining the optimal setting of the experimental factors that produce the maximum (or minimum) value of the response (Khuri and Cornell, 1987:3).

Specific Problem

The goal of this research was to determine if RSM could be effectively used as a calibration technique to estimate groundwater flow parameters.

Research Objectives

To accomplish the stated goal, the following objectives were established:

1. Examine a previously calibrated model that simulates groundwater flow for a cross-section of landfill 10 located on Wright-Patterson Air Force Base, Ohio.

2. Ensure the simulation model implemented on available computer systems produces results similar to those obtained by the developer of the model.

3. Review the available field data associated with the model and establish a calibration criterion.

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4. Attempt to recalibrate the model using the RSM approach.

5. Compare both the effectiveness and efficiency of RSM verses the manual trial-and-error method.

Scope and Limitations

1. This study used an existing two-dimensional, steady-state flow model of a landfill to demonstrate how RSM could be applied to the problem of parameter estimation. The developer of the model used a graphical matching technique to calibrate some of the model's hydraulic parameters. It was assumed the calibrated parameter values were close to optimal. However, no quantitative information on the closeness of calculated response to observed data was available. It was also assumed that the model was valid and adequately represented the physical characteristics of the landfill (including aquifer configuration, external forces exerting on the system, and boundary conditions).

2. This calibration process focused on three of the most commonly adjusted hydraulic parameters and used the calibrated parameter values determined by the developer of the model as the starting point of the investigation.

3. The available field data provided only two points for comparing the observed values with the estimated response from the model.

4. No information was available on the measurement errors associated with the observed head values.

II. Parameter Estimation and the Calibration Process

Introduction

This chapter reviews the parameter estimation techniques used to calibrate groundwater flow models and discusses the use of response surface methodology as a possible parameter estimation procedure. The problem of parameter estimation is set in context by introducing some basic principles of groundwater hydrology, the governing differential equations used to model groundwater flow, and the process used to develop groundwater models. The chapter concludes with an overview of RSM and how it may be useful as a parameter estimation technique.

Groundwater Hydrology

Geologic Framework and Terminology. Any analysis of subsurface fluid flow must take into account the geologic setting. This setting includes the different sediment and rock types in the study area, spatial and temporal relationships among the different subsurface formations, and some sense of the scale of spatial variability. Incomplete characterization of the geologic setting can lead to errors or misinterpretations in groundwater investigations (Smith and Wheatcraft, 1993:6.2).

Aquifers. The aquifer is the most commonly studied subsurface formation in groundwater hydrology. An *aquifer* is a geologic formation which contains water and allows large amounts of water to move through it in response to physical forces. The porous media comprising the aquifer may consist of several sediment and rock types. Regardless of its composition, the portion of the formation which is occupied by solid matter is called the *solid matrix*. The remaining portion is called the *void space* or *pore space*. This pore space is occupied by water, or gases (mainly air and water

vapor), or some combination of water and gases. The *zone of saturation* is defined as the area of a subsurface formation where the pore space is completely filled with water (see Figure 2.1). While the term *subsurface water* is used to denote all the water beneath the surface of the ground, the term *groundwater* refers specifically to the water in the zone of saturation (Bear and Verruijt, 1987:1-4).
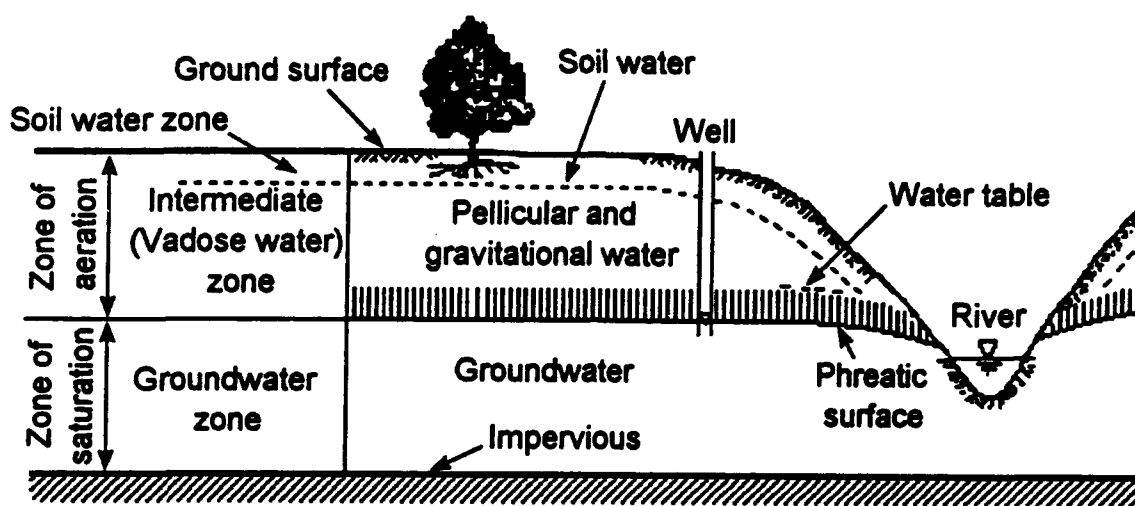
Figure 2.1 Subsurface Moisture Zones (Bear and Verruijt, 1987:4)

Most aquifers can be considered as underground storage reservoirs that receive recharge from rainfall. The rate at which water flows into an aquifer's zone of saturation is known as *rate of recharge*. Only a fraction of the precipitation eventually reaches the zone of saturation and becomes part of the aquifer's groundwater system. Figure 2.2 shows the average annual hydrogeologic budget for Southwest Ohio. While the area receives an average yearly rainfall of 36 inches, the rate of recharge is only about six inches per year.

Hydraulic Properties. To understand and characterize groundwater systems, hydrologists have defined several properties of a porous material. The most

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commonly used definitions are porosity, hydraulic conductivity, permeability. specific

storage, transmissivity, and storage coefficient.
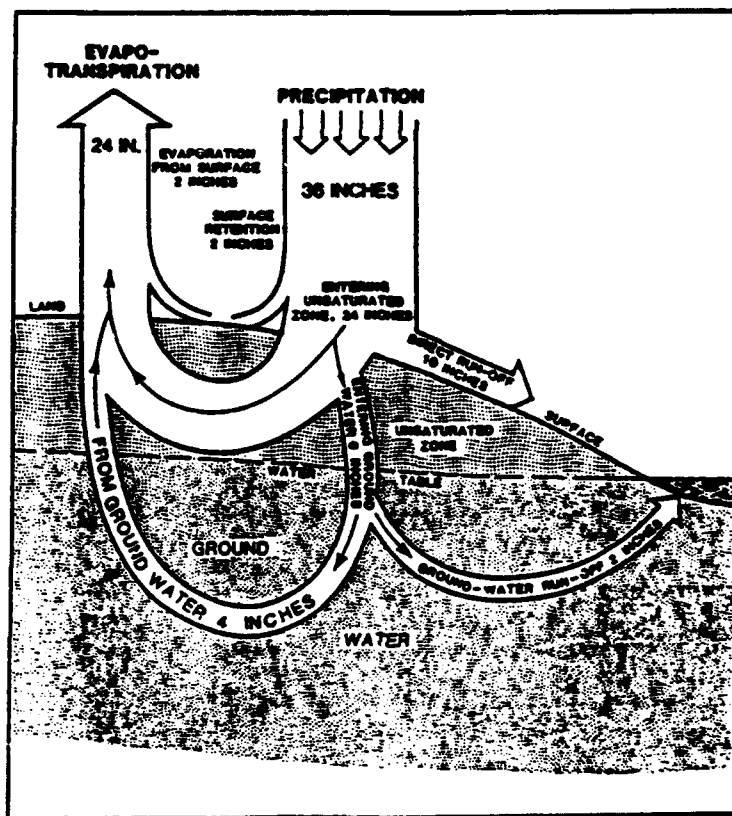
**Figure 2.2 Annual Hydrogeologic Budget for Southwest Ohio
(OSRI Report, 1993:F1.7)**

In the zone of saturation, the *porosity* is a direct measure of the water contained per

unit volume, expressed as a ratio of the volume of pore space to the total volume.

Porosity is a dimensionless number less than one, although it is frequently reported as a

percentage. Table 2.1 shows a range of porosities for a several types of geologic media.

Table 2.1 Representative Values of Porosity (Smith and Wheatcraft, 1993:6.9)

Sediment or Rock Type	Porosity	Sediment or Rock Type	Porosity
Clays	0.40-0.60	Fractured igneous rocks	0.01-0.10
Silts	0.35-0.50	Basalts	0.01-0.25
Fine sands	0.20-0.45	Carbonate mud	0.40-0.70
Coarse sands	0.15-0.35	Dolomite	0.001-0.15
Shales (near-surface)	0.30-0.50	Tertiary limestone	0.20-0.35
Shales (at depth)	0.01-0.10	Paleozoic limestone	0.001-0.10
Sandstones	0.05-0.35	Oolitic limestone	0.01-0.25
Bedded salt	0.001-0.005	Karstified limestone	0.05-0.50
Unfractured igneous rocks	0.0001-0.01	Chalk	0.15-0.45

Hydraulic conductivity (K) is a measure (m/sec) of an aquifer's ability to transmit water. Hydraulic conductivity is a function of both the medium and the fluid and can vary over many orders of magnitude. To separate the effects of the medium from those of the fluid, the *permeability* (k) is defined as

$$k = \frac{K\mu}{\rho g} \qquad (2\text{-}1)$$

where μ (kg/m·sec) is dynamic viscosity of the fluid, ρ (kg/m^3) is fluid density, and g (m/sec^2) is the acceleration due to gravity. Thus, permeability (m^2) is a property of the medium only and describes how well the medium transmits water. When permeability differs according to the direction of flow, the permeability is said to be *anisotropic*. Direction independent permeability is *isotropic*. When permeability is anisotropic, there is always one particular direction, x_p, along which permeability has an absolute maximum value, k_{max}. Somewhere in the plane normal to the maximum direction, there is a direction, x_m, in which permeability has the absolute minimum value, k_{min}. An anisotropic permeability field in two dimensions is completely described by the extreme permeability values, k_{max} and k_{min}, and the angle orienting the principal directions, x_p and x_m, to the x and y directions (see Figure 2.3) (Voss, 1984:28). The maximum permeability value, k_{max}, is often referred to as longitudinal permeability while the

minimum permeability value, k_{min}, is referred to as transverse permeability. The *anisotropic ratio of permeability* is the ratio of longitudinal to transverse permeability. In layered geologic media, this ratio may exceed values as large as 100:1 (Smith and Wheatcraft, 1993:6.9).
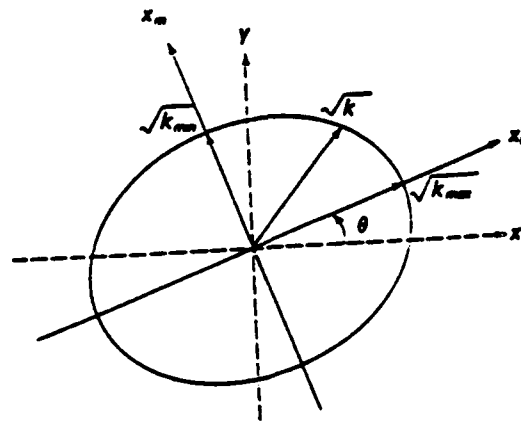
Figure 2.3 Anisotropic Permeability (Voss, 1984:29)

Specific storage (S_s) is defined to be the volume of water released from a unit volume of aquifer per unit change in hydraulic head (see description below). Specific storage (1/m) is a function of both the compressibility of water and the compressibility of the porous medium (Anderson and Woessner, 1992:17).

Transmissivity (T) and storage coefficient (S) are commonly used when modeling two-dimensional horizontal flow through an aquifer with a specified layer thickness. *Transmissivity*, $T = Kb$ (m²/sec), is the product of hydraulic conductivity and the layer thickness; and the *storage coefficient*, $S = S_s b$ (dimensionless), is the product of specific storage and the layer thickness, where b (m) is the thickness of the layer being modeled (Smith and Wheatcraft, 1993:6.12).

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Groundwater Flow.

Hydraulic Potential and Fluid Flux. Understanding the movement of groundwater requires a knowledge of the time and space dependency of the flow, the nature of the porous medium and fluid, and the boundaries of the flow system. Groundwater flows through interconnected void spaces, along microcracks between grain boundaries, and in larger-scale fractures. Groundwater moves in response to differences in fluid pressure and elevation. The driving force is measured in terms of *hydraulic head* (*h*), defined as

$$h = \frac{p}{\rho g} + z \qquad (2\text{-}2)$$

Here p (N/m^3) is the pressure of a fluid with constant density ρ (kg/m^3), g (m/sec^2) is the acceleration due to gravity, and z (m) is the elevation of the measurement point above some reference elevation or *datum*. Hydraulic head (m), also referred to as *piezometric head*, is equal to the mechanical energy per unit weight of the fluid. Groundwater flows from regions where the hydraulic head is higher towards regions where it is lower. Defining *pressure head* as

$$h_p = \frac{p}{\rho g} \qquad (2\text{-}3)$$

leads to

$$h = h_p + z \qquad (2\text{-}4)$$

where z is the *elevation head* (see Figure 2.4). The *water table* is defined as the surface on which the pressure head is equal to zero. Contour maps of hydraulic head are used to infer directions of subsurface fluid flow since flow will be normal to the head contours in an isotropic medium (Smith and Wheatcraft, 1993:6.6).

Darcy's Law. The movement of groundwater is well established by the hydraulic principles reported in 1856 by Henri Darcy. Darcy discovered that the flow rate

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through porous media is proportional to the hydraulic head loss and inversely proportional to the length of the flow path. Darcy's law can be stated as

$$Q = -KA\nabla h = qA \qquad (2\text{-}5)$$

where Q (m³/sec) is the volumetric flow rate, A (m²) is the cross-sectional area of the aquifer, K (m/sec) is the hydraulic conductivity, ∇h (dimensionless) is the gradient in hydraulic head, and q (m/sec) is the specific discharge or flow rate per unit area. The negative sign indicates that fluid flows in the direction of decreasing hydraulic head (Smith and Wheatcraft, 1993:6.7).
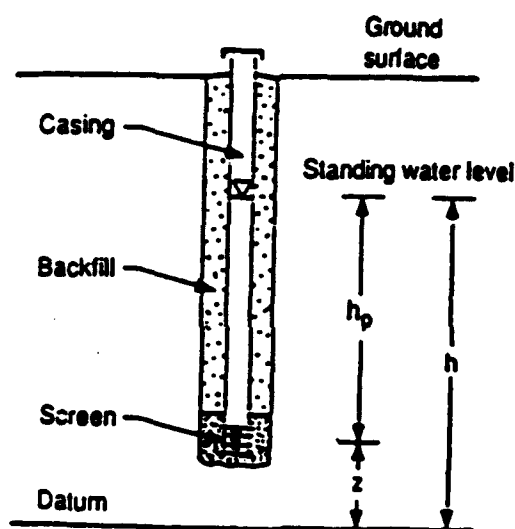
Figure 2.4 Hydraulic Head (Smith and Wheatcraft, 1993:6.7)

Governing Equations. The goal of groundwater modeling is to predict the velocity field from a given set of physical conditions. The *velocity field* is defined by the magnitude and direction of the specific discharge rate. The development of the flow equations is straightforward because all of the flow problems are developed from the same fundamental principle of conservation of fluid or mass. The derivation is traditionally done by referring to a cube of porous material that is large enough to be representative of the properties of the porous medium and yet is small enough so that the

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change of head within the volume is relatively small. This cube of porous material is known as a *representative elementary volume* or REV. Its volume is equal to $\Delta x \Delta y \Delta z$ (see Figure 2.5).
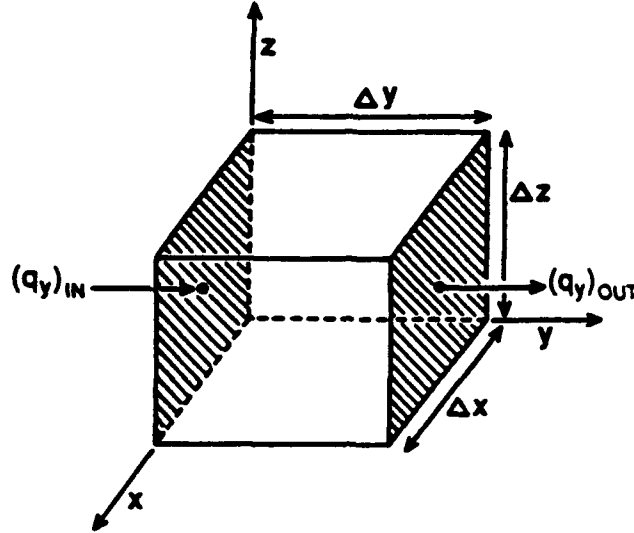
Figure 2.5 Representative Elementary Volume (Anderson and Woessner, 1992:16)

The general conservation equation can be expressed as

$$m_s = m_o - m_i \qquad (2\text{-}6)$$

where m_s is the rate of change in mass storage, m_o is the rate of mass output, and m_i is the rate of mass input. Considering the x-direction only, the change in mass in terms of q can be expressed by

$$m_{s_x} = [q_x(x+\Delta x) - q_x(x)]\Delta y \Delta z \qquad (2\text{-}7)$$

where $q_x(x+\Delta x)$ is the x-component of discharge at $(x+\Delta x)$, $q_x(x)$ is the x-component of recharge at x, and $\Delta y \Delta z$ is the cross sectional area of the REV in the x-direction. Similar reasoning for the y- and z-directions produces

$$m_s = [q_x(x+\Delta x) - q_x(x)]\Delta y \Delta z + [q_y(y+\Delta y) - q_y(y)]\Delta x \Delta z +$$
$$[q_z(z+\Delta z) - q_z(z)]\Delta x \Delta y - R\Delta x \Delta y \Delta z \qquad (2\text{-}8)$$

where R is a volumetric source/sink rate.

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Using the definition of specific storage, the rate of change in storage in the REV is given by

$$m_s = \frac{\Delta V}{\Delta t} = -S_s \frac{\Delta h}{\Delta t} \Delta x \Delta y \Delta z \qquad (2\text{-}9)$$

where ΔV is the change in fluid volume, S_s is the specific storage, and Δh is the change in hydraulic head. Combining Equations 2-8 and 2-9, dividing through by $\Delta x \Delta y \Delta z$, and taking the limit as the volume goes to zero, yields the final form of the water balance equation:

$$-S_s \frac{\partial h}{\partial t} = \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} - R \qquad (2\text{-}10)$$

Because the specific discharge rate, q, cannot be measured directly, Equation (2-10) can not be used to compare analytical results to observed field data. However, hydraulic head can be measured directly in the field by a piezometer and the gradient can be estimated. Darcy's law can then be used to determine the specific discharge. Darcy's law in three dimensions is

$$q_x = -K_x \frac{\partial h}{\partial x},$$

$$q_y = -K_y \frac{\partial h}{\partial y}, \qquad (2\text{-}11)$$

$$q_z = -K_z \frac{\partial h}{\partial z}.$$

Finally, a general and useful form of the governing equation for hydraulic head can be developed by substituting Equation (2-11) into Equation (2-10) yielding:

$$S_s \frac{\partial h}{\partial t} - R = \frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right) \qquad (2\text{-}12)$$

Every problem of flow that can be modeled is described by one or more equations of the form found in Equation (2-12) (Anderson and Woessner, 1992:16-18).

Groundwater Modeling

Overview. Hydrologists are often called upon to predict the response of an aquifer system to proposed changes. The concern may be about the future spatial distribution of water levels, water quality, or cost of a unit volume of water supplied to a customer. The tool most often used to make these predictions is a groundwater flow model of the aquifer system.

In the early 70's, hydrologists used physical models such as sand tanks to simulate groundwater flow directly. Today, most hydrologists use mathematical models to simulate groundwater flow indirectly by means of the governing equations. A conceptual model of the aquifer system includes descriptions of the physical processes, hydraulic properties, and boundary conditions considered relevant to the particular subsurface formation under study. Once formulated, the conceptual model is then translated into a mathematical model. Because of the complexity of groundwater systems, most models are solved numerically rather than analytically. Finite-difference and finite-element methods are the two most commonly used techniques for solving mathematical models in the field of hydrology (Anderson and Woessner, 1992:20). The main features of these methods are:

1. The solution is sought for the numerical values of state variables (hydraulic heads) only at discrete points rather than their continuous variations.

2. The partial differential equations found in the governing equations are replaced by a set of algebraic equations.

3. The solution is obtained for a specified set of numerical values of the various model parameters rather than as general relationships.

4. Computer codes are required to simultaneously solve the very large number of resulting equations (Bear and Verruijt, 1990:16).

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Model Calibration. After the mathematical model has been developed it must be calibrated. Model calibration is the process of adjusting the model's parameters to obtain a reasonable match between observed site-specific data (calibration targets) and results computed by the model (Walton, 1992:35). In effect, the model is calibrated by reproducing a set of historical data with some acceptable level of accuracy. For groundwater flow models, the calibration procedure is generally carried out by varying estimates of hydraulic properties from a set of initial values until the best fit of calculated results to observed data is achieved. Model calibration is synonymous with parameter estimation and is often referred to as solving the inverse problem.

Model calibration is one of the most difficult and time consuming aspects of groundwater modeling (Water Science and Technology Board, 1990:225). In an article on model calibration techniques, Barry Power cites a case that required 500 man-hours and 80 simulation runs to estimate one parameter in finite-element model with 222 nodes (Power and Barns, 1993:9). Some of the reasons parameter estimation is so difficult are:

1. Too few observations are available to compute stable estimates of statistics such as mean and variance.

2. Results of point sampling are often biased because a large amount of data does not necessarily allow computation of nearly true or effective values of a parameter and its variance. For example, permeability values from core analyses often are not representative of regional values, because flow through large fractures is not reproduced by core analyses.

3. Observed values are subject to numerous sources of error such as mismeasuring water levels, clogging of the slots or screen in the measuring devices, and inaccurate reporting (Cooley and Naff, 1989:4).

The techniques for parameter estimation are numerous and range from simple graphical curve fitting to complex statistical estimation algorithms. Excellent reviews of

the various procedures can be found in (Yeh, 1986) and (Carrera, 1988). Historically, the techniques have been divided into two major categories: (1) manual trail-and-error procedures and (2) automated or optimization methods that minimize an objective function.

Manual Trial-and-Error Calibration. In manual trial-and-error calibration, the parameters are assigned initial values based on the limited information available. During calibration, the parameter values are adjusted sequentially in an attempt to match simulated heads to the calibration targets. The modeler makes the parameter adjustments based on his or her expertise and knowledge of the model and the area being simulated. No matter how the method is applied, it has several inherent deficiencies:

1. It typically requires tens to hundreds of model runs (Anderson and Woessner, 1992:232).

2. No methodology exists to guarantee that simulations will proceed in a direction that could lead to an optimal set of parameter estimates.

3. It is difficult to determine if the best set of parameter estimates has been reached.

4. The parameters are usually calibrated one at a time, overlooking possible interaction effects.

5. The method is labor intensive (therefore expensive), frustrating (therefore often left incomplete) and subjective (therefore biased) (Carrera and Neuman, 1986:199).

Manual trail-and-error was the first technique to be used and is still the preferred method in practice despite its many drawbacks (Keidser and Rosbjerg, 1991:2219).

Automated Calibration. To address some of the above deficiencies, researchers have developed several automated calibration techniques. Automated calibration is performed using specially developed codes that use either a direct or indirect approach to solve for the parameter estimates (Anderson and Woessner, 1992:233). In a direct approach, the unknown parameters are treated as dependent

2-12

variables in the governing differential equations and heads are treated as independent variables. To use this approach, the head values must be specified at all points within the system. Since heads are known only at points where there are observation wells, the head at all other points must be estimated. For this reason and because direct solutions are prone to instability[1], the direct method has received little attention and is not often used. The main advantage of the direct method is that it does not require repeated simulation runs.

The indirect approach is similar to performing manual trial-and-error calibrations in that the simulation is executed repeatedly. However, rather than adjusting the parameters based on the modeler's opinion, some objective function is used to make the adjustments to the parameters. The objective function is usually some measure of how close the calculated heads are to the observed heads. Many of the objective functions, also called calibration criteria, can be written in a general form as

$$\text{minimize} \quad \| h - \hat{h} \| \qquad (2\text{-}13)$$

where h is the set of observed heads and $\hat{h}$ is the set of calculated heads (Loaiciga and Church, 1990:645). The double vertical bars represent a norm or measure of agreement. Some of the calibration criteria that have been used in the past are (1) minimization of the sum of squared deviations (i.e., least squares criterion), (2) minimization of the maximum absolute deviation, and (3) minimization of the sum of absolute deviations. Least squares is one of the most commonly used criteria primarily because of its computational convenience. Methods used to optimize (minimize) the objective function include (1) linear programming, (2) quadratic programming, (3) Gauss-Newton method, and (4) gradient search methods. Most studies have used either a Gauss-Newton or gradient search method (Yeh, 1986:98).

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[1] A solution is instable if small changes (or errors) in head values cause large changes in the parameter estimates.

Automated techniques provide a systematic approach to model calibration. They usually require fewer simulation runs, are less subjective, and provide statistical information on the accuracy of the parameter estimates. Despite these advantages, they are still not widely used. Perhaps the primary reason is inertia on the part of groundwater modelers. However, some have criticized automated techniques for failing to recognize, or treat adequately, the problems of nonidentifiability[2], nonuniqueness[3], and instability (Carrera and Neuman, 1986:200).

One strategy which some of the automated techniques touch on but do not seem to take full advantage of is response surface methodology.

Response Surface Methodology

Response surface methodology (RSM) comprises a group of statistical techniques for empirical model building and model exploitation. RSM (or "The methodology"), first introduced by Box and Wilson in 1951 and later developed by Box, Hunter, and Draper, consists of: (1) design of experiments, (2) regression analysis, and (3) model exploitation or optimization (Cornell, 1990:1). One of the primary goals of RSM is to find the best value of the estimated response. In the case of parameter estimation for groundwater models, the response would usually be the residual sum of squares between observed and calculated heads, and the goal would be to find the set of parameter values which produce the minimum error. Figure 2.6 shows an example of a sum of squares error surface where the model has two parameters (β_1 and β_2).

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[2]A parameter is said to be nonidentifiable if the model output is not sensitive to it. If a parameter is nonidentifiable, then regardless of the value assigned to the parameter, the model will produce the same output.
[3]Even if all the parameters are identifiable, the solution to the minimization problem may be nonunique. This is usually associated with multiple local minima.
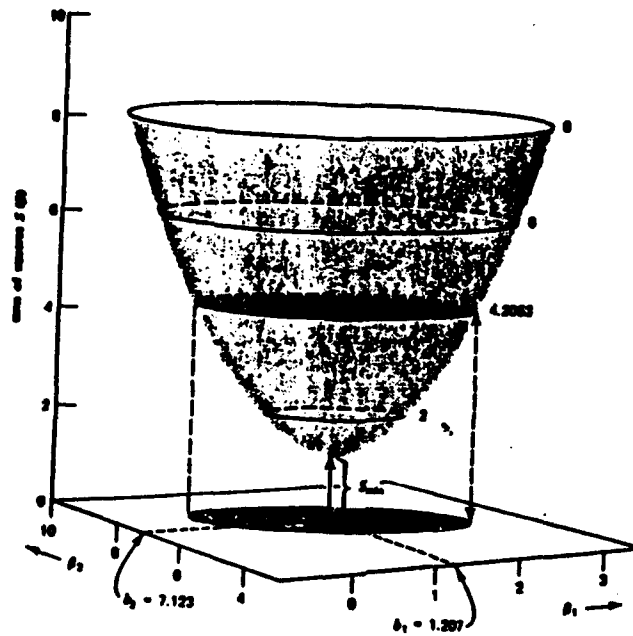
Figure 2.6 Sum of Squares Error Surface (Box and others, 1978:463)

Experimental Design. The first step in setting up an experimental design is
deciding which input variables (ξ_i) to study. Usually, the researcher has numerous
possible input variables to consider. In applying RSM to groundwater flow models, the
decision involves which of the model parameters to estimate as part of the calibration
process. Often for convenience and computational efficiency, the input variables, ξ_i, are
transformed into coded or standardized variables, x_i. Generally, the following linear
transformation is used:

$$x_i = \frac{\xi_i - \xi_{i0}}{S_i} \qquad (2\text{-}14)$$

where ξ_{i0} is the center of the region of interest and S_i is the half range of the region. The
next step in setting up a design determines the levels of the input variables included in the

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design. For groundwater flow models, a reasonable range of values for certain parameters can be determined from observed data. For example, if an aquifer is made up of fine sands, a reasonable range for the levels of porosity would be 0.20–0.45 (see Table (2.1)). The final step specifies the experimental arrangement or design. One of the basic designs is a two-level factorial (2^k) design. In such a design, each of the k variables occurs at just two levels (± 1 in coded space). Factorial designs in general have the following useful properties:

1. They allow numerous comparisons to be made and therefore facilitate model creation and criticism.

2. They provide estimates whose variances are as small, or nearly as small, as those provided by any other design occupying the same space.

3. They give rise to simple calculations (Box and Draper, 1987:106).

Two-level factorial designs are often used to estimate models with main effects and n-factor interactions. To build a quadratic model, a 3^k factorial arrangement can be used, but the more efficient central composite designs (CCDs) and Box-Behnken designs are generally preferred. A central composite design consists of

1. the 2^k vertices of a k-dimensional cube where the factor levels are coded so that the design center is at $(0,0, \ldots ,0)$. The values of the coded variables in this factorial portion are $(\pm 1, \pm 1, \ldots, \pm 1)$;

2. the center point, $n_0 = (0,0, \ldots ,0)$ and;

3. the $2k$ vertices $(\pm \alpha, 0, 0, \ldots ,0)$, $(0, \pm \alpha, 0, \ldots .0)$, $\ldots$, $(0,0, \ldots ,0, \pm \alpha)$ of a k-dimensional star (Cornell, 1990:52).

Figure 2.7 shows a central composite design for three variables.

One feature often incorporated into a CCD is rotatability. In a rotatable design, the accuracy of prediction of the response depends only on its distance from the center of the design, producing a variance function that is spherical or nearly spherical. Rotatability is

2-16

achieved by assigning appropriate α-values. A general formula used to achieve

rotatability in a full factorial design is:

$$\alpha = \left(\frac{2^k r_c}{r_s} \right)^{\frac{1}{4}}$$
(2-15)

where k is the number of factors, r_c is the number of observations at the cube points, and

r_s is the number of observations at the star points (Box and Draper, 1987:488).

Axial or "star" points
$(\pm a, 0, 0)$
$(0, \pm a, 0)$
$(0, 0, \pm a)$

2^3 or "cube" points
$(\pm 1, \pm 1, \pm 1)$

"Cube" + "star"
+ center points
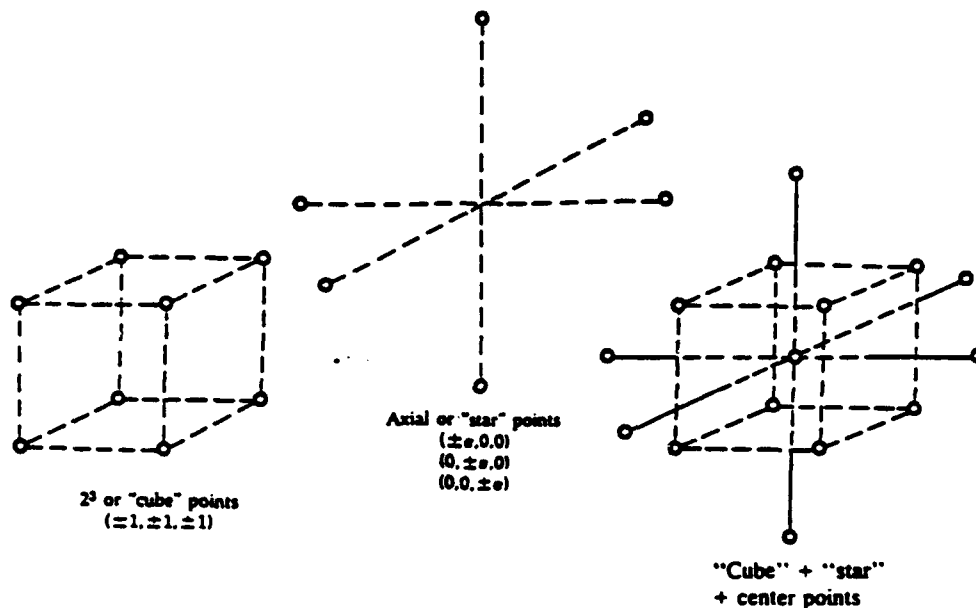
Figure 2.7 Central Composite Design (Cornell, 1990:53)

Another feature often incorporated into experimental designs is orthogonality. In an

orthogonal two-level design, each column in the design matrix is orthogonal to every

other column. This design results in a diagonal variance-covariance matrix and produces

a smaller joint confidence region than a nonorthogonal design (Box and Draper,

1987:78). Because of the axial points in a central composite design, the column

corresponding to the constant term will not be orthogonal with those corresponding to the

2-17

quadratic terms. For second order designs, orthogonality refers to the absence of correlation between the quadratic terms.

Box-Behnken designs are a subset of the class of 3^k designs. By leaving out the corner points from the full 3^k design, they require fewer runs. Box-Behnken designs are often used because they require only three levels for each variable and not five as in a CCD (Cornell, 1990:60).

Regression Analysis. After selecting a design, the groundwater model can be solved and the residual sum of squares computed for each design point. Regression analysis techniques can then be applied to this data to develop an empirical model of the error surface. For a discussion of regression analysis techniques including the method of least squares and analysis of variance, see any standard text on regression analysis (Draper and Smith, 1981; Montgomery and Peck, 1982).

Optimization. The third area of RSM is searching for optimal conditions. To accomplish this task, it is useful to know what type of surface the model represents. For second order models with only one variable, a simple curve is produced. Figure 2.8 shows a curve with a minimum. If the model had included two variables, some of the possible surfaces include: a simple minimum (or maximum), a saddle, a stationary ridge, or a rising ridge (see Figure 2.9).
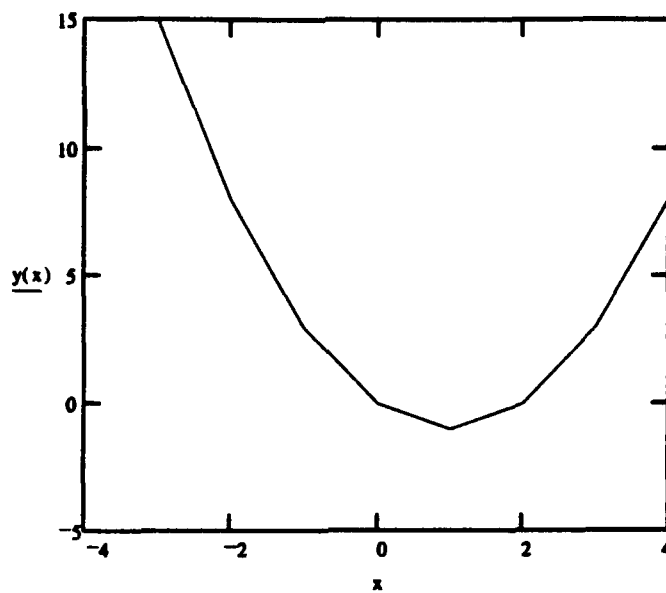
Figure 2.8 Simple Curve for Second Degree Polynomial in One Variable
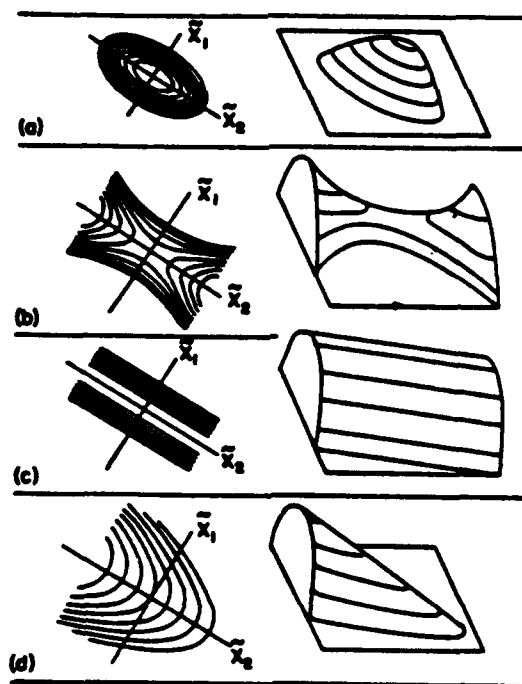
Figure 2.9 Ridge Systems for Second Degree Polynomials in Two Variables
(Box and Draper, 1987:347)

For second-order models with three variables, only the iso-response contours associated
with the fitted surface can be examined. Figure 2.10 shows some of these contours. It
was expected the iso-response contours of the residual sum of squares error surface would
look something like Figure 2.10a.
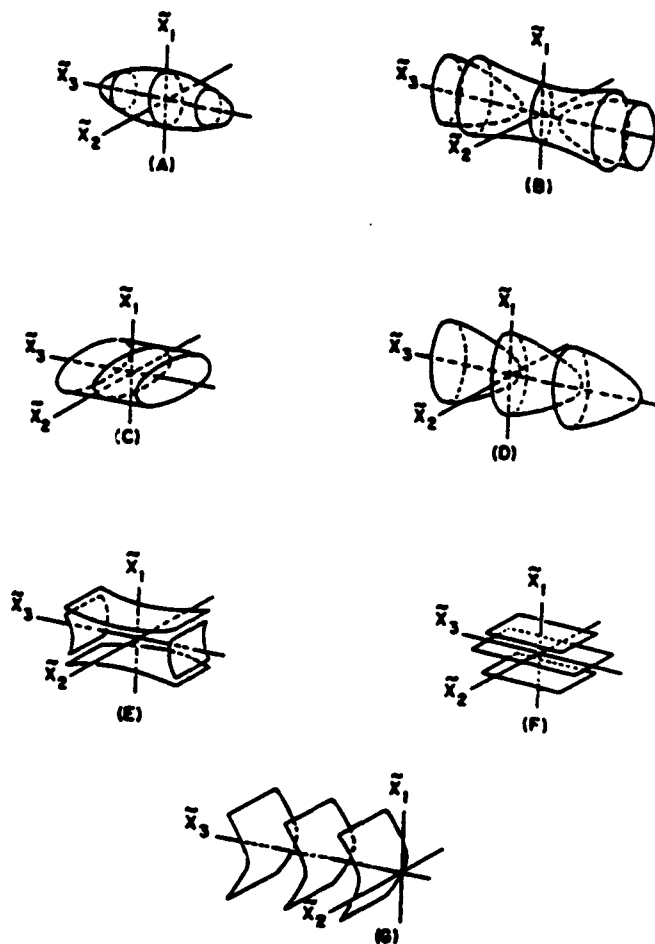
**Figure 2.10 Contour Systems for Second Degree Polynomials in Three Variables
(Box and Draper, 1987:350)**

2-20

There are two basic methods used to search for optimal conditions: (1) a calculus based approach, and (2) canonical analysis. In the calculus based approach, the partial derivative of the function is taken with respect to each factor and each partial derivative is set equal to zero. A stationary point (if one exists) can then be found by solving the resulting set of equations. The nature of the surface at the stationary point can be determined by examining the partial second derivatives. The partial second derivatives are presented in the Hessian matrix:

$$H = \begin{bmatrix} \dfrac{\partial^2 \hat{y}}{\partial x_1^2} & \cdots & \dfrac{\partial^2 \hat{y}}{\partial x_1 x_k} \\ \vdots & \cdots & \vdots \\ \dfrac{\partial^2 \hat{y}}{\partial x_k x_1} & \cdots & \dfrac{\partial^2 \hat{y}}{\partial x_k^2} \end{bmatrix} \qquad (2\text{-}16)$$

If $x^T H x \leq 0 \; \forall x$ then the function is concave and will have a simple maximum at its stationary point. If $x^T H x \geq 0 \; \forall x$ then the function is convex and will have a simple minimum at its stationary point. If neither of the above is true, then a simple maximum or minimum does not exist.

The other method used to analyze second-order models is canonical analysis. A canonical analysis involves rotating the coordinate axes to remove all cross-product terms and when appropriate, translating the coordinate axes to coincide with the stationary point. Performing a canonical analysis simplifies the model, allows local optimum to be easily identified, and makes the description of the surface relatively straightforward. The details of canonical analysis are available in several references (Box and draper, 1987; Khuri and Cornell, 1987; Box and others, 1978)

III. Results and Analysis

Introduction

The primary objective of this research was to determine if response surface methodology (RSM) could be used as a parameter estimation technique in groundwater flow modeling. To test this hypothesis, an attempt was made to calibrate an existing two-dimensional, steady-state flow model using the RSM approach. The model was reviewed and tested on three different computer platforms. Simulation results were compared to the output obtained by the developer of the model. The available field data was examined and a calibration criterion established. Three of the model's hydraulic parameters were then selected for calibration and an experimental design built. Using the method of least squares, a regression model of the error surface was developed and analyzed.

Landfill Model

Examining the efficacy of using RSM as a parameter estimation technique for groundwater flow models required a model to calibrate. Rather than developing a new model, this research conducted experiments on an existing model.

Model Description. The particular model used in this study simulated groundwater flow and solute transport for a cross-section of landfill 10 located on Wright-Patterson Air Force Base, Ohio. The cross-section, referred to as JDb in the developer's report, is oriented in a generally east-west direction and extends approximately 1100 feet from test pit WP-LF10-TP12 to monitoring well WP-LF10-MW04 (see Figure 3.1). As shown by the lines of equal potentiometric head, the groundwater flow within this area was nearly all vertical. The porous matrix was composed mostly of fine sand, gravelly sand, and clay.

3-1
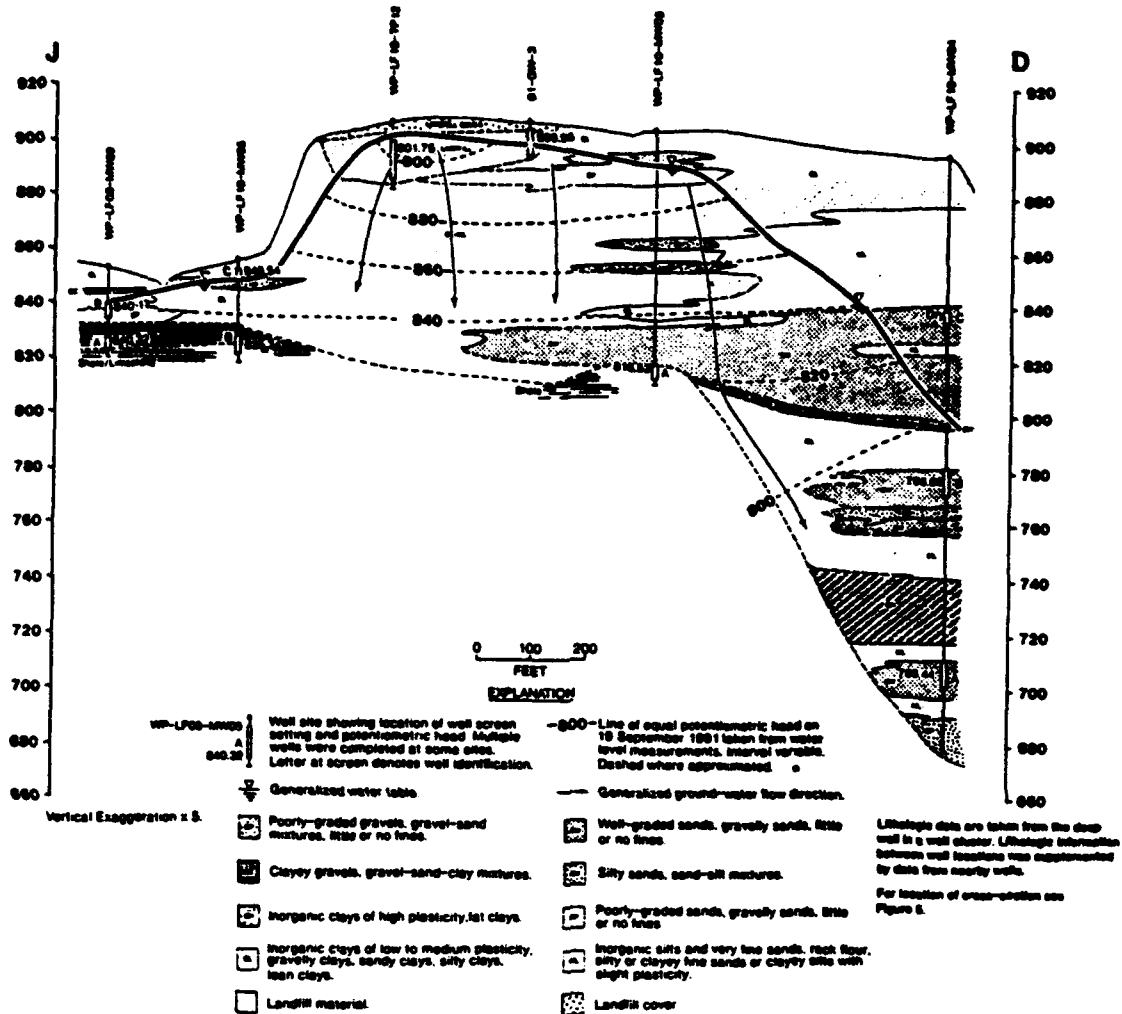
Figure 3.1 Cross-Section JD of Landfill 10 (OSRI Report, 1993:U-19)

The numerical model SUTRA (Saturated-Unsaturated Transport) was used to simulate the groundwater flow and solute transport of the landfill. SUTRA is a computer program developed by the United States Geological Survey (USGS) and written in ANSI-STANDARD FORTRAN-77. The version of SUTRA used in this study, V-0690-2D, was released in June of 1990. The program employs a two-dimensional hybrid finite-element and integrated finite-difference method to approximate the governing differential

3-2

equations (Voss, 1984:3). This approximation method divides the cross-sectional aquifer domain into a single layer of contiguous blocks, called finite elements. Flow parameters and variables which vary from point to point in the aquifer are approximated elementwise, nodewise, or cellwise (see Figure 3.2). Elementwise approximation implies that a parameter has a constant value over each element, although it may differ from element to element. Nodewise approximation results in a continuous surface of values with linear change between adjoining nodes. Cellwise approximation is similar to elementwise approximation but each cell is centered on a node, not on an element. The grid for cross-section JDb (Figure 3.3) contained 1320 elements and 1416 nodes. Constructing a finite element grid is a time-consuming process and one of the reasons an existing model was used in this study.
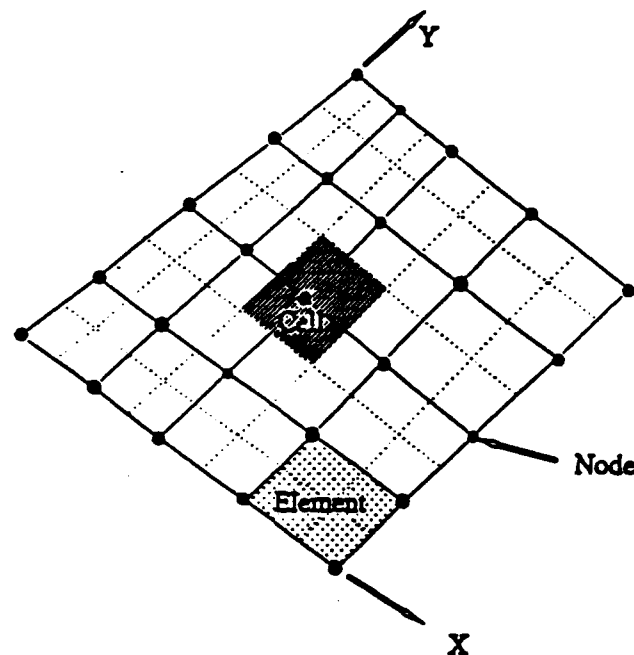
Figure 3.2 Graphical Representation of Elements, Cells, and Nodes
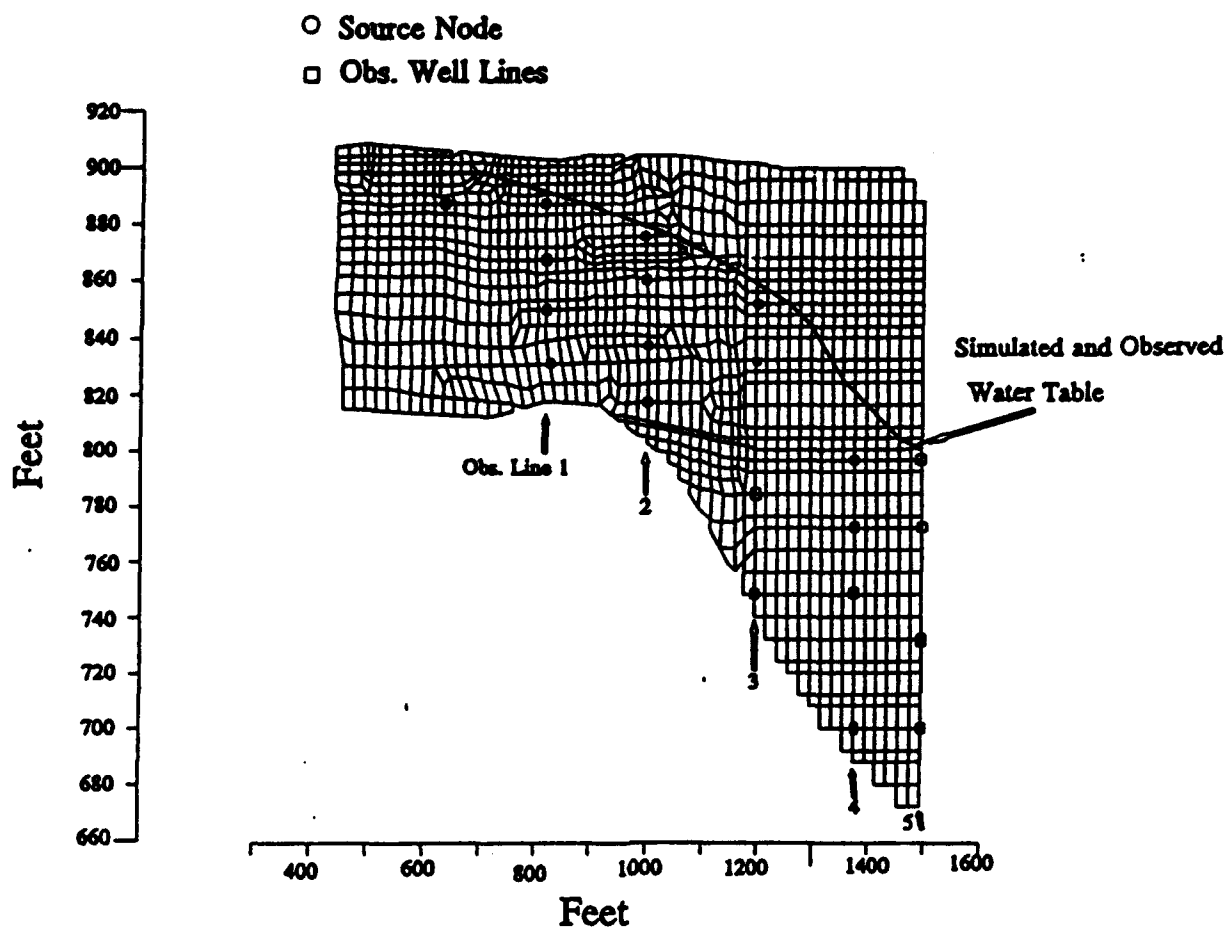
Figure 3.3 Cross-section JDb; Finite Element Mesh

Model Execution. SUTRA requires two input files for operation. The primary
input file contains all the data necessary for the simulation except the initial conditions.
The second input file contains the initial conditions of pressure and concentration. As the
primary output, SUTRA provides fluid pressures and solute concentrations, as they vary
with time, everywhere in the simulated subsurface system (Voss, 1984:3). The model
used in this investigation was run in steady-state mode and therefore the fluid pressures
did not vary with time. The model also calculated solute concentrations, but these values
were not relevant to this study. Copies of the primary input file and output file for the

landfill model were available for use in this study. The initial conditions input file was not available, but was created from the output file since the output file also lists the initial conditions.

SUTRA can be compiled and executed under most operating systems and on most computers. The developers of the landfill model used the Lahey fortran compiler and a 486 microcomputer. The Lahey compiler was not available for use in this study. The model was compiled under Microsoft Fortran version 5.1 and execution was attempted on both a 386 and 486 microcomputer. On both machines, the program would not execute properly. The model was successfully compiled and executed on a VAX/VMS machine and under the UNIX operating system. The output from the VAX/VMS and UNIX runs matched. However, there were significant differences between the results obtained locally and the output supplied by the developer of the model. The pressure differences at the 1416 nodes ranged from zero to $8.9E03$ N/m^2. Some possible explanations for these discrepancies include the different compilers and computer platforms used and the possibility of different initial conditions. However, these differences should not affect the study since the baseline will be the results of the local runs.

Calibration Criterion

The developer of the model used manual trial-and-error and graphical matching techniques to calibrate the model. The developer stated,

> Water-level data available from monitoring wells in the vicinity of Landfills 8 and 10 were used to aid in calibrating the numerical models. Hydraulic parameters, particularly the degree of anisotropy in hydraulic conductivity values and the rates of recharge, were adjusted in the model until water levels simulated by the model resembled water levels observed in the monitoring wells. ... results can only be tentative until rigorous parameter calibration and model validation is performed. Herein, the model is used to simulate plausible hypotheses and aid in understanding the physics of the system. Provided that the uncertainty of model parameters is recognized, this understanding can be helpful in assessing the risk of contaminant migration. (OSRI Report, 1993:5-49,U-7)

3-5

No quantitative information on the closeness of observed data to calculated results was provided.

The most commonly used calibration targets are observed hydraulic heads. Head measurements from four observation wells were taken on three separate occasions over an eight month period (see Table 3.1). The three observations taken at each well were averaged to produce a single calibration target per well. It was assumed these average values represented steady-state conditions. No information was available on the error associated with the head measurements.

Table 3.1 Head Observations

| Well Number | Hydraulic Head (ft) | | | |
	7 May 91	19 Sep 91	14 Jan 92	Average
01-GW-3	904.05	899.98	906.40	903.48
WP-LF10-MW03A	818.68	818.53	818.61	818.61
WP-LF10-MW04A	797.80	796.44	796.58	796.94
WP-LF10-MW04B	801.26	799.66	799.66	800.19

After examining the model, it was discovered that the pressures at the nodes corresponding wells WP-LF10-MW04A and WP-LF10-MW04B were set to constant values as boundary conditions for the model. Consequently, only the observations for wells 01-GW-3 and WP-LF10-MW03A were available as calibration targets. Since SUTRA calculates fluid pressures instead of heads, the fluid pressures for the two remaining observations were determined by

$$p = (h - z)\rho g \tag{3-1}$$

3-6

where h (m) is the observed hydraulic head, z (m) is the elevation above datum, ρ (kg/m^3) is the fluid density, and g (m/sec^2) is the acceleration due to gravity. For these calculations, the values for fluid density (1000 kg/m^3) and gravitational acceleration (9.8 m/sec^2) were the same as those used in the landfill model. The elevation values used were 274.015 m and 249.326 m for wells 01-GW-3 and WP-LF10-MW03A respectively. These values were estimated from the cross-sectional diagram shown in Figure 3.1. The drawing is to scale and the estimates were obtained by using the middle of the well symbol as a reference point. The resulting approximations seemed reasonable when compared to the finite-element mesh which gives elevation and range values for each node. The drawing is to scale and The results of converting the observed hydraulic heads to fluid pressures appear in Table 3.2.

Table 3.2 Observed Fluid Pressure

Well Number	Fluid Pressure (N/m^2)
01-GW-3	1.33810563E+04
WP-LF10-MW03A	1.81336727E+03

There are several objective functions or criteria that could be used to determine the best parameter estimates. Among these are minimization of the maximum absolute deviation, minimization of the sum of absolute deviations, and minimization of the sum of squares of the deviations (or least squares). Because of its widespread use and computational convenience, it was decided to use the least squares method. The equation for calculating the residual sum of squares over n observation points is

$$RSS = \sum_{i=1}^{n} (p_i - \hat{p}_i)^2 \tag{3-2}$$

where p_i is the observed pressure (calibration target) and $\hat{p}_i$ is the pressure calculated by the model.

To establish a quantitative value for how close the model was initially calibrated, the developer's output was compared to the observed fluid pressures. Table 3.3 shows the comparison. The RSS indicated that while the overall results may match the observed water-level, individual comparisons may show large discrepancies.

Table 3.3 Quantitative Value of Calibration

Well/Node Number	Observed Fluid Pressure (N/m^2)	Developer's Results (N/m^2)	Residual Sum of Squares
01-GW-3/244	1.33810563E+04	-2.38676270E+04	8.9116592E+09
WP-LF10-MW03A/539	1.81336727E+03	8.85554844E+04	

Input Variables

The model contains eleven main hydraulic parameters that must be specified: fluid density, porosity, permeability (longitudinal and transverse), fluid viscosity, porous matrix compressibility, fluid compressibility, residual saturation, parameters of the saturation-pressure and permeability relationships, and rate of recharge (OSRI Report, 1993:U-25, U-29). Some of these parameters, such as fluid density, fluid viscosity, porous matrix compressibility, fluid compressibility, and residual saturation, can generally be adequately determined from either the literature or from field and laboratory experiments. Values for the others must usually be determined through a calibration process. To demonstrate the RSM technique, three parameters (porosity, transverse permeability, and rate of recharge) were selected as parameters to be calibrated. This

choice seemed reasonable since these were the same parameters the developer of the landfill model calibrated.

Porosity. The porous matrix of the cross-sectional layer being modeled consists of inorganic clays, gravelly clays, sandy clays, silty clays, lean clays, inorganic silts, very fine sands, rock flour, well-graded sands, and gravelly sands (see Figure 3.1). As shown in Table 2.1, typical ranges of porosity for these sediments are: clays (0.40-0.60), silts (0.35-0.50), fine sands (0.20-0.45), and course sands (0.15-0.35). The developers of the model used 0.40 as the value for porosity (OSRI Report, 1993:U-25). This study examined porosity values from 0.05 to 0.75.

Transverse Permeability. Transverse permeability, when different from longitudinal permeability, gives an indication of the degree of anisotropy of the system. The value(s) for transverse permeability cannot be determined directly from field sampling. The developers of the model initially assumed an isotropic system (1:1 ratio of longitudinal to transverse permeability), but later calibrated the model with an anisotropic ratio of 100:1 (OSRI Report, 1993:U-30). This study examined transverse permeabilities that produced anisotropic ratios ranging from 500:1 to 55.6:1.

Rate of Recharge. According to Figure 2.2 the average amount of yearly rainfall reaching the groundwater in southwest Ohio is four inches (not including run-off). When the developer of the model assumed an isotropic system, the rate of recharge was calibrated to an unreasonable value of 18.6 inches per year (OSRI Report, 1993:U-30). When the model was run as an anisotropic system (100:1), the rate of recharge was calibrated to four inches per year matching the expected value. The actual parameter value entered into the model is computed by averaging the yearly rate over the surface area (approximately 1100 square feet). The inflow is then specified at each of the surface nodes. For example, the four inches per year equates to 2.0E-07 kg/sec for each of the

surface nodes. This study examined rates of recharge ranging from 2.03E-09 kg/sec to 3.98E-07 kg/sec, which equate to 0.04 and 7.96 inches per year, respectively.

Coded Variables. The final calibrated value for each parameter, as determined by the model developer, was used as the center point for the variables in the design region. The three variables were transformed into coded space by:

$$x_1 = \frac{\xi_1 - 0.4}{0.208}, \quad x_2 = \frac{\xi_2 - 0.01}{0.00476}, \quad \text{and } x_3 = \frac{\xi_3 - 2.00E - 07}{1.177E - 07}. \tag{3-3}$$

Experimental Design

Since a sum of squared residuals was used as the calibration criteria for this study (see Equation (3-2)), a design that would allow the creation of a quadratic model was needed. A central composite design (CCD) was chosen over a 3^k design because CCDs are more efficient, requiring fewer simulation runs. Table 3.4 shows the CCD design in both uncoded and coded form. The design is a composite of a two-level factorial design represented by the eight cube points ($\pm 1, \pm 1, \pm 1$), combined with the center point (0, 0, 0), and augmented with six star or axial points ($\pm 1.682, 0, 0$), (0, $\pm 1.682, 0$), (0, 0, ± 1.682). The cube points allow the estimation of first order and two-way interaction effects while the center and star points allow the estimation of pure quadratic effects. The star points were chosen using Equation (2-15) to make the design rotatable. Since SUTRA is a deterministic model, only one run was conducted at each of the design points.

Regression Analysis

The results of executing the groundwater flow model at each of the design points are shown in Table 3.5. Table 3.6 lists the residual sum of squares and the sum of signed differences. The first item to note is the large values for the residuals (on the order of 10^9 and 10^{10}). Upon obtaining these values, the calculations involving the calibration targets were verified and found to be correct.

3-10

Table 3.4 Central Composite Design

Uncoded			Coded			
Porosity, ξ_1	Transverse Permeability, ξ_2	Rate of Recharge, ξ_3	Porosity, x_1	Transverse Permeability, x_2	Rate of Recharge, x_3	
0.192	0.00524	8.23E-08	-1	-1	-1	
0.608	0.00524	8.23E-08	1	-1	-1	
0.192	0.01476	8.23E-08	-1	1	-1	
0.608	0.01476	8.23E-08	1	1	-1	Cube
0.192	0.00524	3.18E-07	-1	-1	1	Points
0.608	0.00524	3.18E-07	1	-1	1	
0.192	0.01476	3.18E-07	-1	1	1	
0.608	0.01476	3.18E-07	1	1	1	
0.400	0.01000	2.00E-07	0	0	0	Center Point
0.050	0.01000	2.00E-07	-1.682	0	0	
0.750	0.01000	2.00E-07	1.682	0	0	
0.400	0.00200	2.00E-07	0	-1.682	0	Axial
0.400	0.01800	2.00E-07	0	1.682	0	Points
0.400	0.01000	2.03E-09	0	0	-1.682	
0.400	0.01000	3.98E-07	0	0	1.682	

Table 3.5 Results from CCD

Run	Coded Variables			Fluid Pressure	
	Porosity, x_1	Transverse Permeability, x_2	Rate of Recharge, x_3	Node 244	Node 539
1	-1	-1	-1	-2.24948402E+04	7.11774274E+04
2	1	-1	-1	-2.24948402E+04	7.11774274E+04
3	-1	1	-1	-2.45766239E+04	9.96608946E+04
4	1	1	-1	-2.45766239E+04	9.96608946E+04
5	-1	-1	1	-2.19215516E+04	7.11849601E+04
6	1	-1	1	-2.19215516E+04	7.11849601E+04
7	-1	1	1	-2.42890995E+04	9.96709079E+04
8	1	1	1	-2.42890995E+04	9.96709079E+04
9	0	0	0	-2.36630370E+04	8.84435243E+04
10	-1.682	0	0	-2.36630370E+04	8.84435243E+04
11	1.682	0	0	-2.36630370E+04	8.84435243E+04
12	0	-1.682	0	-2.48210152E+04	1.05434369E+05
13	0	1.682	0	-1.88335580E+04	5.12087129E+04
14	0	0	-1.682	-2.33534517E+04	8.84513403E+04
15	0	0	1.682	-2.39864018E+04	8.84351885E+04

3-11

Table 3.6 RSS and Sum of Signed Deviations

Run	Residual Sum of Squares (RSS)	Sum of Signed Deviations
1	6.098452785E+09	-3.348816369E+04
2	6.098452785E+09	-3.348816369E+04
3	1.1014924088E+10	-5.988984718E+04
4	1.1014924088E+10	-5.988984718E+04
5	6.058692013E+09	-3.406898499E+04
6	6.058692013E+09	-3.406898499E+04
7	1.0995138893E+10	-6.018738489E+04
8	1.0995138893E+10	-6.018738489E+04
9	8.877048953E+09	-4.958606379E+04
10	8.877048953E+09	-4.958606379E+04
11	8.877048953E+09	-4.958606379E+04
12	1.2196710264E+10	-6.541893029E+04
13	3.477681542E+09	-1.718073138E+04
14	8.855562446E+09	-4.990346509E+04
15	8.899666835E+09	-4.925436319E+04

Some possible explanations for the large discrepancies between observed and calculated pressures include:

1. The boundary conditions of the model may not be correctly specified.

2. The two nodes from the finite-element mesh (244 and 539) may not correspond exactly to the locations of the observation wells.

The second item that can be easily seen from Table 3.5 is that porosity has no effect on the RSS. Comparing the runs where the porosity value goes from low (-1) to high (+1) while the other parameter remain unchanged clearly shows that porosity has no effect on the output of the model. This may be a case of nonidentifiablity as discussed in chapter 2. Despite the unusually large residuals and porosity not effecting the output, an empirical model of the error surface was developed. As discussed earlier, it was believed a quadratic model of the form

$$g(x,\beta) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 +$$
$$\beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 \qquad (3-4)$$

would be needed to adequately represent the error surface. The statistical software package, SAS, was used to analyze the RSS data. The regression procedure was run with the input variables in their coded form. The best model produced was

$$\hat{y} = 8.892616142 \cdot 10^9 + 2.1516519152 \cdot 10^9 x_2 - 3.65644160 \cdot 10^8 x_2^2 \qquad (3\text{-}5)$$

As expected, the porosity variable was not included in the model. Also, the rate of recharge was determined to have no significant effect on the output, leaving only the transverse permeability variable in the model. The associated analysis of variance for the model is shown in Table 3.7. Even though this is the "best" model for the data, as evidenced by the large F and R-Square values, the mean square error and the standard errors for the estimates were extremely large. Also the coefficient of variation (C.V.), which expresses the ratio of the root mean square error to the mean response, was high. All these indicators imply that the model has a high degree of variability and is of low precision.

Table 3.7 Analysis of Variance for Equation 3-5

Source	DF	Sum Of Squares	Mean Square	F Value	Prob>F
Model	2	8.8042932E19	4.4021466E19	8575.668	0.0001
Error	12	6.1599585E16	5.1332987E15		
C Total	14	8.8104532E19			

Root MSE	7.1646704E07	R-Square	0.9993	
Dep Mean	8.5596789E09	Adj R-Square	0.9992	
C.V.	0.83703			

Variable	DF	Parameter Estimate	Standard Error	T for H0: Param=0	Prob>|T|
Intercept	1	8.892616142E09	2.6646318E07	333.728	0.0001
x_2	1	2.516519152E09	1.9386560E07	129.807	0.0001
x_2^2	1	-3.65644160E08	2.1062304E07	-17.360	0.0001

A graph of the regression model represented by Equation (3-5) is shown in Figure 3.4. The area between the two vertical lines is the experimental region. This graph shows that the optimal value for transverse permeability was not in the design region and that lowering the value of transverse permeability produces lower values for the residual sum of squares. The graph also indicates that the anisotropic ratio of 100:1, which the developer of the landfill model considered to be close to optimal, was not warranted.
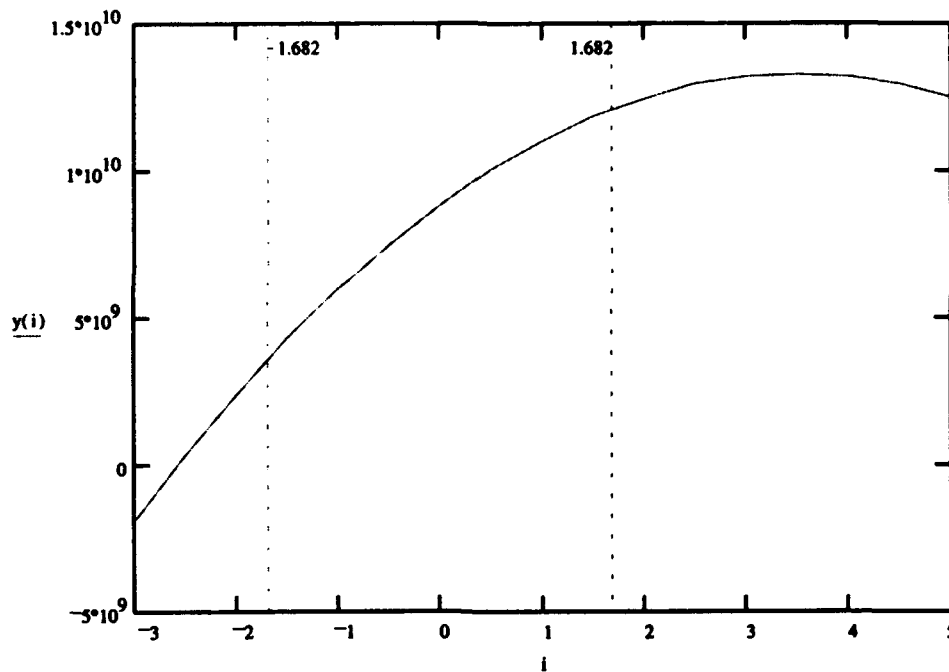

Figure 3.4 Plot of Regression Model (Equation 3-5)

Given the poor utility of the results, the basic assumptions of this study were reviewed. The first assumption was that the calibrated parameter values determined by the developer of the landfill model were close to optimal. However, Table 3.3 showed that,

at least for the two observation points available, a significant difference existed. Another assumption was that porosity and rate of recharge would effect the model's response. The results in Table 3.5 and the absence of these parameters from the regression model demonstrated that they had little or no effect. Based on the review of these assumptions, the lack of additional data, and the low precision of the regression model, it was decided further investigation with the RSM technique would be pointless in this case. While no definite conclusions about the effectiveness of RSM as a parameter estimation technique could be made from the results of this study, the potential still remains. The next step in this process would be to test the technique on a standardized or hypothetical model and possibly using a screening design to determine which parameters have the most effect of the model's response.

IV. Conclusions and Recommendations

Conclusions

The goal of this research was to determine if response surface methodology (RSM) could be used to estimate groundwater flow parameters. This study was motivated by the need for a systematic approach to groundwater flow model calibration. Currently, manual trial-and-error techniques are the most commonly used calibration methods.

An attempt was made to calibrate an existing two-dimensional, steady-state flow model using RSM. The developer of the landfill model used a graphical technique to calibrate several of the model's hydraulic parameters. The developer's approach consisted of matching predicted water-table levels to observed water-table levels. The developer stated the levels were close but no quantitative information on the closeness of fit was provided. The RSM approach was applied using the developer's calibrated parameter values as the starting point of the investigation and a residual sum of squares was used as the calibration criterion. Following the developer's lead, porosity, transverse permeability, and rate of recharge, were the three hydraulic parameters which were to be estimated. After executing the landfill model at each of the design points, the residual sum of squares were calculated. The residuals had an order of magnitude of 10^9 and 10^{10} indicating a significant difference between the observed and calculated fluid pressures. Also the regression model of the error surface revealed a large amount of variability in the data. Only the transverse permeability parameter was included in the regression model indicating that, at least in the area of the design region, porosity and rate of recharge had little or no effect on the landfill model's output.

This investigation started with the assumption that the parameter values determined by the landfill model developer were close to optimal and that the three hydraulic parameters

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selected for calibration would be significant. The assumptions turned out not to be valid. Because of these bad assumptions, low precision of the regression model, and lack of additional data, the investigation was terminated. No definite conclusions about the effectiveness of RSM as a parameter estimation technique could be made from the results.

Recommendations

The following are some recommendation for extending this research:

1. Rather than using a groundwater flow model of a real system, the RSM technique could be tested against a hypothetical or synthetic model. An example of using a hypothetical model can be found in an article by Chu, Strecker, and Lettenmaier (Chu and others, 1987).

2. A preliminary screening design could be used to determine which hydraulic parameters have the most effect on the response surface and then those parameters used for further study.

3. An investigation could be conducted to compare the results of using different calibration criteria, such as minimization of the absolute differences, minimization of the maximum difference, and a weighted least squares.

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13. ABSTRACT (Maximum 200 words)

This thesis examined the use of response surface methodology (RSM) as a parameter estimation technique in the field of groundwater flow modeling. Using RSM, an attempt was made to calibrate three hydraulic parameters (porosity, transverse permeability, and rate of recharge) of an existing two-dimensional, steady-state flow model. The model simulated groundwater flow for a portion of landfill 10 located on Wright-Patterson Air Force Base, Ohio. The model had previously been calibrated by graphical matching observed water-levels to predicted water-levels. Using the parameter values from the earlier calibration effort as a starting point, a central composite design was developed and the simulation executed at each design point. A residual sum of squares function was used as the calibration criteria and an empirical model of the error surface was developed. Of the three hydraulic parameters, only transverse permeability had a significant effect on the response. The regression model also indicated the response had a high degree of variability. A graph of the regression equation revealed no local optima within the design region indicating the initial parameter estimates may not have been warranted.

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